The Bias-Variance Tradeoff: A Deep Dive

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Understanding the Problem Setup

The Learning Problem: A Real-World Example

Definition: Our Scenario

Goal: Predict housing prices based on house area

Example: The True Relationship

Unknown to us: There exists a true function $f_{\theta_{\text{true}}}$ that perfectly relates area to price:

$$y_t = f_{\theta_{\mathsf{true}}}(x_t)$$



The 3 Sources of Error

Any prediction made is affected by 3 sources of error:

- Noise
- Bias
- Variance

A relation between **price** and **size** will be affected by other factors that we have not considered or cannot be perfectly captured. Such factors would include:

- the condition of the house (cannot be measured perfectly)
- sale prices of other houses in the neighborhood (measurements that have biases in themselves)

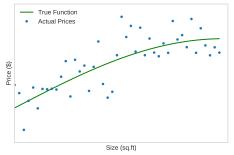
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- the condition of the house (cannot be measured perfectly)
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Because of this, data is inherently noisy.

This is **not** a property of data but rather an **irreducible error**.

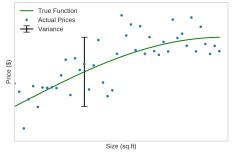
This is **not** a property of data but rather an **irreducible error**. This error can be captured by the error term ϵ which causes the final value of the house to follow the equation: $y_t = f_{\theta_{\text{true}}}(x_t) + \epsilon_t$



Modeling the relation

This noise can be assumed to be mean-centered around 0 with spread called the variance of the noise.

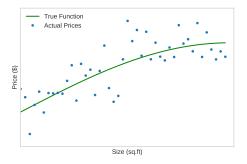
This causes y_t to become mean centered around the true relation.



Modeling the relation

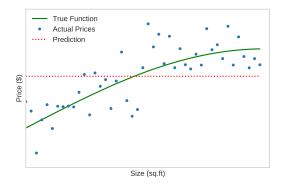
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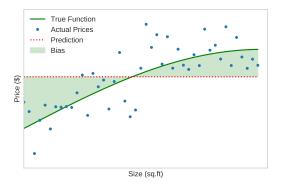
An example dataset

To understand this, let us take an example where we try to learn the relation that models the *Price* and *Size* of a house using a *constant* function.



An example dataset

So the bias in this scenario looks something like this:

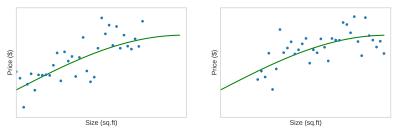


An example dataset

But it is important to understand that there are a large number of different datasets possible for a given situation, with each having their individual fits.

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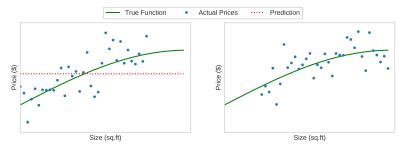
Assume that we have two datasets of houses sold.



Two Datasets from same relation

But it is important to understand that there are a large number of different datasets possible for a given situation, with each having their individual fits.

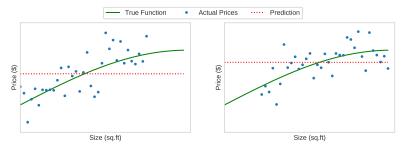
If we try to fit a constant function to them.



Two Datasets from same relation

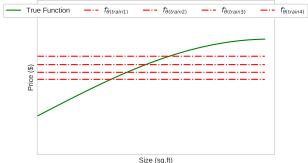
But it is important to understand that there are a large number of different datasets possible for a given situation, with each having their individual fits.

We see that they show different predictions.



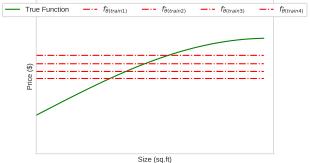
Two Datasets from same relation

Doing so for all possible size N training sets we get



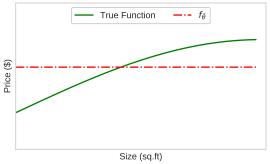
Size (sq.ft)
Fits on different training sets

Doing so for all possible size N training sets we get A way of consolidating all these possible fits is to calculate an average fit that is weighted by how likely they are to appear.



Fits on different training sets

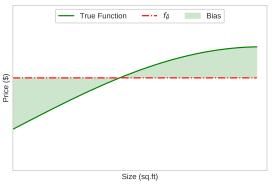
Averaging all the fits (as in this scenario all datasets are equally likely) we get the average fit.



Average fit on all different training sets

Bias Contribution



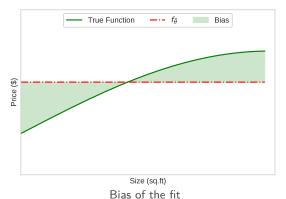


Bias of the fit

Bias Contribution

$$\mathsf{Bias}(x) = f_{\theta_{\mathsf{true}}}(x) - f_{\bar{\theta}}(x)$$

It is a measure of how flexible the fit is in capturing $f_{\theta_{\text{true}}}(x)$

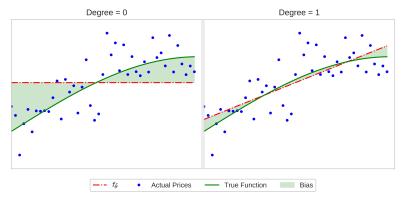


Bias Contribution: Effect of Complexity

As we increase the complexity of the fit

⇒ fit becomes more flexible

⇒ bias decreases



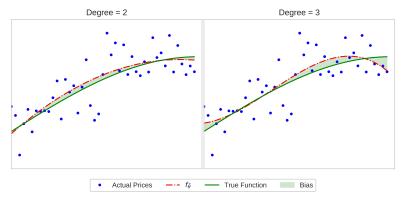
Effect of degree on Bias of the fit

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Effect of degree on Bias of the fit

Bias: Calculating the Bias

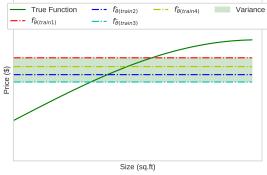
Bias calculation for a model is at the core a calculation of the area under a curve.

Therefore, finding the bias for a model in the range (a, b) is the calculation of the integral:

$$\int_{a}^{b} |f_{\bar{\theta}}(x) - f_{\theta(\mathsf{true})}(x)| dx$$

Variance

Variance of the fit is a measure of the variation in the fits when trained across different training sets.

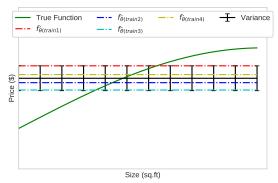


Variance of the fit

Variance Contribution

For Low Complexity

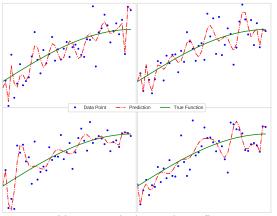
- ⇒ variations between curves are less
- ⇒ Variance is less



Variance of the low complexity fits

Variance Contribution

For High Complexity we see very high variation



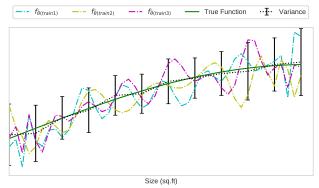
Variance in high complexity fits

Variance Contribution

For High Complexity

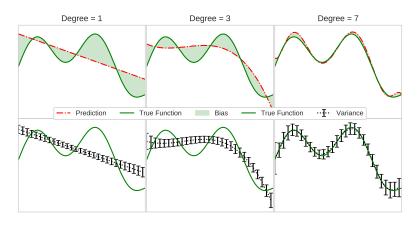
⇒ high variation

⇒ Variance is high



Variance of the high complexity fits

The Bias-Variance Trade off



Variance in high complexity fits

The Bias-Variance Trade off

Plot Graph - 3:06 Variance and the bias-variance trade off

Mathematically

Formulating the Error of a Model

Measuring the goodness of a Model

To measure the goodness of a model, we have to understand how well it can predict the behavior of the phenomenon it is trying to model.

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Therefore, it is important to measure performance averaged over all possible training sets (of size N).

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Therefore, it is important to measure performance averaged over all possible training sets (of size N).

$$E_{\text{training set}}[\text{error of } \hat{\theta}(\text{training set})]$$

gives a measure of the average error by doing an expectation of the errors of all possible training sets of size N.

Expected Prediction Error at a point

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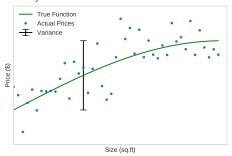
Therefore, $E_{train}[at a point x_t] = f(noise, bias, variance)$

Formally defining the 3 sources of error: Noise

Noise is an **irreducible error** captured by the error term ϵ . The equation of the relation becomes $y_t = f_{\theta(true)}(x_t) + \epsilon_t$

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Variance in the noise

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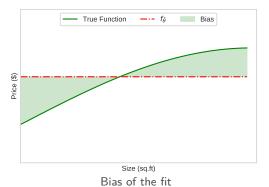
That is, it can be denoted by $\epsilon_t \sim \mathcal{N}(0, \sigma^2)$

Formally defining the 3 sources of error: Bias

Bias is a measure of how flexible the fit is in capturing the true function $f_{\theta_{\mathrm{true}}}(x)$

$$\mathsf{Bias}(x_t) = f_{\theta_{\mathsf{true}}}(x_t) - f_{\bar{\theta}}(x_t)$$

where $f_{\bar{\theta}}$ denotes the average fit over all datasets.



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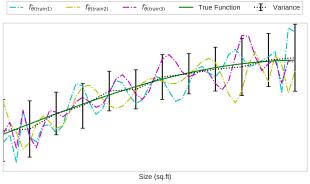
$$\mathsf{Bias}(x_t) = f_{\theta_{\mathsf{true}}}(x_t) - f_{\bar{\theta}}(x_t)$$

where $f_{ar{ heta}}$ denotes the average fit over all datasets.

As $f_{\bar{\theta}}$ denotes the average fit over all datasets, it can be expressed by $f_{\bar{\theta}}(x_t) = E_{\text{train}}[f_{\hat{\theta}}(x_t)]$

Formally defining the 3 sources of error: Variance

Variance of the fit is a measure of the variation in the fits when trained across different training sets.



Variance of a fit

Formally defining the 3 sources of error: Variance

Variance of the fit is a measure of the variation in the fits when trained across different training sets.

Variance of the fit can be defined by

$$\operatorname{var}(f_{\hat{\boldsymbol{\theta}}}(x_t)) = E_{\operatorname{train}}[(f_{\hat{\boldsymbol{\theta}}}(x) - f_{\bar{\boldsymbol{\theta}}}(x_t))^2]$$

where $f_{\hat{\theta}}(x) - f_{\bar{\theta}}(x_t)$ denotes the deviation that a specific fit has from the average.

Now we will see how, $E_{train}[\text{at a point } x_t] = \sigma^2 + [\text{bias}(f_{\hat{\theta}}(x_t))]^2 + \text{var}(f_{\hat{\theta}}(x_t))$ where, given a training set, the parameters $\hat{\theta}$ of the fit are learned as $f_{\hat{\theta}}$ and, the prediction at a point x_t for the model trained on that training set is $f_{\hat{\theta}}(x_t)$

Prediction Error at a point x_t can be calculated using the squared loss function.

Prediction error at
$$x_t = (y_t - f_{\hat{\theta}(train)}(x_t))^2$$

To find the "Expected Prediction Error" at a point x_t we average out the prediction error at that point over all possible learned models. This can be done by finding the expectation of prediction error for that point over all possible training datasets (train) and labels for that point (y_t) .

Expected prediction error at
$$x_t = E_{train,y_t}[(y_t - f_{\hat{\theta}(train)}(x_t))^2]$$

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= $E_{train,y_t}[((y_t - f_{\theta(true)}(x_t)) + (f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t)))^2]$

Expected prediction error at
$$x_t = E_{train,y_t}[(y_t - f_{\hat{\theta}(train)}(x_t))^2]$$

$$= E_{train,y_t}[(\underbrace{(y_t - f_{\theta(true)}(x_t))}_{\text{a}} + \underbrace{(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))}_{\text{b}})^2]$$

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$$= E_{train,y_t}[(a + b)^2]$$

Expected prediction error at
$$x_t = E_{train,y_t}[(y_t - f_{\hat{\theta}(train)}(x_t))^2]$$

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$$= E_{train,y_t}[(a+b)^2]$$

$$= E_{train,y_t}[a^2 + 2ab + b^2]$$

$$E_{train,y_t}[a^2] = E_{train,y_t}[(y_t - f_{\theta(true)}(x_t))^2]$$

$$\begin{split} E_{train,y_t}[a^2] &= E_{train,y_t}[(y_t - f_{\theta(true)}(x_t))^2] \\ &\qquad \qquad \text{(Since there is no dependence on training set)} \\ &= E_{y_t}[(y_t - f_{\theta(true)}(x_t))^2] \end{split}$$

$$\begin{split} E_{train,y_t}[a^2] &= E_{train,y_t}[(y_t - f_{\theta(true)}(x_t))^2] \\ &\quad (\because \text{ there is no dependence on training set}) \\ &= E_{y_t}[\underbrace{(y_t - f_{\theta(true)}(x_t))^2}_{\epsilon_t^2}] \\ &= E_{y_t}[\epsilon_t^2] \end{split}$$

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$$E_{train,y_t}[ab] = E_{train,y_t}[(y_t - f_{\theta(true)}(x_t))(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))]$$

$$E_{train,y_t}[ab] = E_{train,y_t}[\underbrace{(y_t - f_{\theta(true)}(x_t))}_{\epsilon_t}(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))]$$

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$$\begin{split} E_{train,y_t}[ab] &= E_{train,y_t}[\underbrace{(y_t - f_{\theta(true)}(x_t))}_{\epsilon_t}(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))] \\ &= E_{train,y_t}[\epsilon_t(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))] \\ &(\because \epsilon_t \text{ and } (f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t)) \text{ are independent}) \\ &= \underbrace{E_{train,y_t}[\epsilon_t]}_{=0} \times E_{train,y_t}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))] \\ &= 0 \end{split}$$

$$(\text{By definition } \epsilon_t \text{ has mean } 0)$$

 $E_{train \ v_t}[ab] = 0....(Eqn. 3)$

$$\begin{split} E_{train,y_t}[ab] &= E_{train,y_t}[\underbrace{(y_t - f_{\theta(true)}(x_t))}_{\epsilon_t}(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))] \\ &= E_{train,y_t}[\epsilon_t(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))] \\ &(\because \epsilon_t \text{ and } (f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t)) \text{ are independent}) \\ &= \underbrace{E_{train,y_t}[\epsilon_t]}_{=0} \times E_{train,y_t}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))] \\ &= 0 \end{split}$$

$$(\text{By definition } \epsilon_t \text{ has mean } 0)$$

$$E_{train,y_t}[b^2] = E_{train,y_t}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))^2]$$

$$\begin{split} E_{train,y_t}[b^2] &= E_{train,y_t}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \\ (f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t) \text{ is independent of } y_t) \\ &= E_{train}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \end{split}$$

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$$\begin{split} E_{train,y_t}[b^2] &= E_{train,y_t}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \\ (f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t) \text{ is independent of } y_t) \\ &= E_{train}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \\ &= MSE(f_{\hat{\theta}(train)}(x_t)) \\ E_{train,y_t}[b^2] &= MSE(f_{\hat{\theta}(train)}(x_t)) \dots (Eqn. 4) \end{split}$$

From Eqn. 1, 2, 3 and 4, we get,

Expected prediction error at $x_t = \sigma^2 + MSE(f_{\hat{\theta}(train)}(x_t))$

Now, we will further simplify the MSE term into bias and variance.

$$MSE(f_{\hat{\theta}(train)}(x_t)) = E_{train}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))^2]$$

$$\begin{aligned} MSE(f_{\hat{\theta}(train)}(x_t)) &= E_{train}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \\ &= E_{train}[((f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t)) + (f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t)))^2] \end{aligned}$$

$$MSE(f_{\hat{\theta}(train)}(x_t)) = E_{train}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))^2]$$

$$= E_{train}[(\underbrace{(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))}_{\alpha} + \underbrace{(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))}_{\beta})^2]$$

$$\begin{aligned} & \mathit{MSE}(f_{\hat{\theta}(train)}(x_t)) = E_{train}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \\ &= E_{train}[(\underbrace{(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))}_{\alpha} + \underbrace{(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))}_{\beta})^2] \\ &= E_{train}[(\alpha + \beta)^2] \end{aligned}$$

$$MSE(f_{\hat{\theta}(train)}(x_t)) = E_{train}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))^2]$$

$$= E_{train}[(\underbrace{(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))}_{\alpha} + \underbrace{(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))}_{\beta})^2]$$

$$= E_{train}[(\alpha + \beta)^2]$$

$$= E_{train}[\alpha^2 + 2\alpha\beta + \beta^2]$$

$$\begin{split} & \mathit{MSE}(f_{\hat{\theta}(train)}(x_t)) = E_{train}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \\ &= E_{train}[(\underbrace{(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))}_{\alpha} + \underbrace{(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))}_{\beta})^2] \\ &= E_{train}[(\alpha + \beta)^2] \\ &= E_{train}[\alpha^2 + 2\alpha\beta + \beta^2] \\ &\quad (\mathsf{Using Linearity of Expectation}) = E_{train}[\alpha^2] + 2E_{train}[\alpha\beta] + E_{train}[\beta^2] \\ &\dots (\mathsf{Eqn. 5}) \end{split}$$

$$E_{train}[\alpha^2] = E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))^2]$$

$$\begin{split} E_{train}[\alpha^2] &= E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))^2] \\ &= E_{train}[(f_{\theta(true)}(x_t) - E_{train}[f_{\hat{\theta}(train)}(x_t)]^2] \end{split}$$

$$\begin{split} E_{train}[\alpha^2] &= E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))^2] \\ &= E_{train}[(f_{\theta(true)}(x_t) - E_{train}[f_{\hat{\theta}(train)}(x_t)]^2] \\ &= E_{train}[bias(f_{\hat{\theta}}(x_t))^2] \end{split} \tag{By definition of bias}$$

$$\begin{split} E_{train}[\alpha^2] &= E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))^2] \\ &= E_{train}[(f_{\theta(true)}(x_t) - E_{train}[f_{\hat{\theta}(train)}(x_t)]^2] \\ &= E_{train}[bias(f_{\hat{\theta}}(x_t))^2] \qquad \qquad \text{(By definition of bias)} \\ &= bias(f_{\hat{\theta}}(x_t))^2 \\ &\quad (\because \text{ bias is not a function of training data)} \end{split}$$

$$\begin{split} E_{train}[\alpha^2] &= E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))^2] \\ &= E_{train}[(f_{\theta(true)}(x_t) - E_{train}[f_{\hat{\theta}(train)}(x_t)]^2] \\ &= E_{train}[bias(f_{\hat{\theta}}(x_t))^2] \qquad \qquad \text{(By definition of bias)} \\ &= bias(f_{\hat{\theta}}(x_t))^2 \\ &\quad (\because \text{bias is not a function of training data)} \\ E_{train}[\alpha^2] &= bias(f_{\hat{\theta}}(x_t))^2 \dots (Eqn. 6) \end{split}$$

$$\begin{aligned} &E_{train}[\alpha\beta] \\ &= E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))] \end{aligned}$$

$$\begin{split} &E_{train}[\alpha\beta] \\ &= E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))] \\ &= E_{train}[bias_t \times (f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))] \end{split}$$

$$\begin{split} &E_{train}[\alpha\beta] \\ &= E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))] \\ &= E_{train}[bias_t \times (f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))] \\ &= bias_t \times E_{train}[f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t)] \\ &(\because bias_t \text{ is not a function of training data}) \end{split}$$

$$\begin{split} &E_{train}[\alpha\beta] \\ &= E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))] \\ &= E_{train}[bias_t \times (f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))] \\ &= bias_t \times E_{train}[f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t)] \\ &(\because bias_t \text{ is not a function of training data}) \\ &= bias \times \left(E_{train}[f_{\bar{\theta}}(x_t)] - E_{train}[f_{\hat{\theta}(train)}(x_t)] \right) \end{split}$$

$$\begin{split} &E_{train}[\alpha\beta] \\ &= E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))] \\ &= E_{train}[bias_t \times (f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))] \\ &= bias_t \times E_{train}[f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t)] \\ &(\because bias_t \text{ is not a function of training data}) \\ &= bias \times \left(E_{train}[f_{\bar{\theta}}(x_t)] - E_{train}[f_{\hat{\theta}(train)}(x_t)] \right) \\ &= bias \times (f_{\bar{\theta}}(x_t) - f_{\bar{\theta}}(x_t)) \\ &(\because f_{\bar{\theta}}(x_t) = E_{train}[f_{\hat{\theta}(train)}(x_t)) \end{split}$$

$$E_{train}[\beta^2] = E_{train}[(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))^2]$$

$$\begin{aligned} E_{train}[\beta^2] &= E_{train}[(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \\ &= E_{train}[(f_{\hat{\theta}(train)}(x_t) - f_{\bar{\theta}}(x_t))^2] \end{aligned}$$

$$\begin{split} E_{train}[\beta^2] &= E_{train}[(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \\ &= E_{train}[(f_{\hat{\theta}(train)}(x_t) - f_{\bar{\theta}}(x_t))^2] \\ &= E_{train}[(f_{\hat{\theta}(train)}(x_t) - E_{train}[(f_{\hat{\theta}(train)}(x_t)])^2] \\ & (\because f_{\bar{\theta}}(x_t) = E_{train}[(f_{\hat{\theta}(train)}(x_t)]) \end{split}$$

$$\begin{split} E_{train}[\beta^2] &= E_{train}[(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \\ &= E_{train}[(f_{\hat{\theta}(train)}(x_t) - f_{\bar{\theta}}(x_t))^2] \\ &= E_{train}[(f_{\hat{\theta}(train)}(x_t) - E_{train}[(f_{\hat{\theta}(train)}(x_t)])^2] \\ & (\because f_{\bar{\theta}}(x_t) = E_{train}[(f_{\hat{\theta}(train)}(x_t)]) \\ &= variance(f_{\hat{\theta}}(x_t)) \end{split}$$

$$\begin{split} E_{train}[\beta^2] &= E_{train}[(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \\ &= E_{train}[(f_{\hat{\theta}(train)}(x_t) - f_{\bar{\theta}}(x_t))^2] \\ &= E_{train}[(f_{\hat{\theta}(train)}(x_t) - E_{train}[(f_{\hat{\theta}(train)}(x_t)])^2] \\ & (\because f_{\bar{\theta}}(x_t) = E_{train}[(f_{\hat{\theta}(train)}(x_t)]) \\ &= variance(f_{\hat{\theta}}(x_t)) \\ E_{train}[\beta^2] &= variance(f_{\hat{\theta}}(x_t)).......(Eqn. 8) \end{split}$$

From Eqn. 1 - 8, we get,

Expected prediction error at x_t

$$= \sigma^2 + MSE(f_{\hat{\theta}(train)}(x_t))$$

$$=\sigma^2+\mathit{bias}(f_{\hat{ heta}}(x_t))^2+\mathit{variance}(f_{\hat{ heta}}(x_t))$$